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First-principles investigation of armchair boron nitride nanoribbons for sensing PH_3 gas molecules

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ABSTRACT

The present work exhibits density functional theory (DFT) based first-principles calculations to explore the sensing properties of bare armchair boron nitride nanoribbons (ABNNR) for PH_3 gas molecules. Edges of the ribbon were considered as the sites of possible adsorption with two different configurations i.e. adsorption at one edge and adsorption at both edges of the ribbon. It is revealed that B atoms of the ribbons are more energetically favorable sites for the adsorption of PH_3 molecules as compared with N atoms. The adsorption of PH_3 affects the electronic properties of nanoribbons. One edge PH_3 adsorbed ribbons are metallic whereas in both edges PH_3 adsorption, the band gap is decreased than that of bare ribbon. The changes in electronic properties caused by PH_3 adsorption are further supported by the current–voltage (*I–V*) characteristics of the considered configurations. The results show that ABNNR can serve as a potential candidate for PH_3 sensing applications.

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1. Introduction

The successful synthesis of first purely 2-D crystal, graphene [1], worked as a milestone in the research area of material science and was honored by Noble prize of physics in 2010. The importance of the graphene (one atom thick hexagonal arrangement of C atoms) is due to its remarkable physical properties and potential for various technological applications [1–6]. Inspired from the potential of

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this organic 2-D layer, the scientific committee is actively engaged in the synthesis of various other low dimensional materials and exploration of their novel properties [7–9]. These serious efforts have shown the existence of various 2-D materials including boron nitride (BN), MoS_2, WS_2, ZnO, CuO and TiO_2 [7,10–14]. The nanotubes of various materials such as carbon, SiC, BN, AlN, TiO_2 and ZnO [15–21] have also been studied for the adsorption of different gas molecules. Further, the nanoribbons of these 2-D materials exhibit remarkable potential for various technological applications [22–25]. The nanoribbons are quasi 1-D structures whose electronic properties are highly dependent upon the ribbon width as well as the geometry of the edges [26–30]. Experimental realization of graphene nanoribbons [31] made it possible to explore their real life applications. In nanoribbons, each edge atom has an unsaturated dangling bond. The presence of these dangling bonds makes the ribbon edges more reactive as compare to its central part. Thus, nanoribbons enjoy the edge reactivity with 100% exposure of its constituent atom to the environment which makes them a potential candidate for sensor applications. Previous results show that the band gap of zigzag BN nanoribbons (ZBNNR) continually decreases as the ribbon width increases. On the other hand, the band gap of armchair BN nanoribbons (ABNNR) exhibit oscillatory behavior with respect to their width [29]. There exists plenty of literature studying the sensing properties of graphene or GNR [32–35], however, similar work with the other nanoribbons is still almost ignored. The search of novel materials for hydrogen storage, adsorption of natural gases and sensing of hazardous gases is always an issue of great importance for the scientific community. Motivated from this, in the present manuscript, we have performed first-principles investigations to reveal the sensing properties of BNNR for toxic gases. To be concise, here we have considered only ABNNR. Particularly, we have explored the most stable adsorption configuration and the corresponding changes in the electronic and transport properties of ABNNR. Such calculations will be useful to develop efficient nano-sensors in near future based upon BNNR.

2. Computational details

All the present results were obtained using first-principles approach within the banner of density functional theory (DFT). We used Atomistix ToolKit Virtual NanoLab (ATK-VNL) [36] for the calcula-

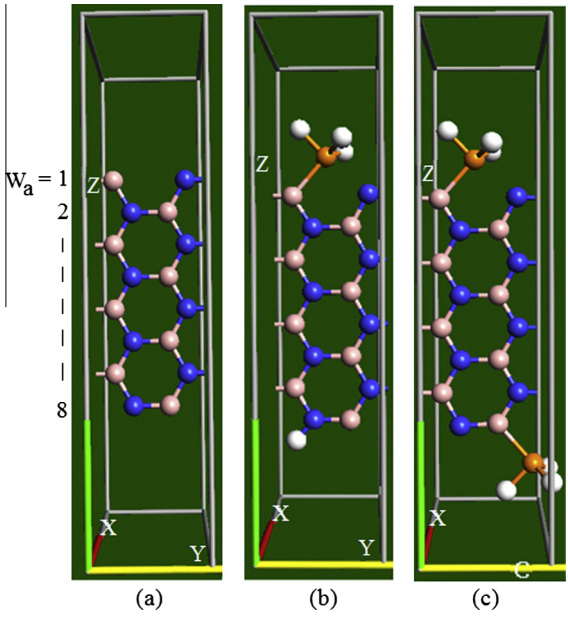

Fig. 1. The schematic models of supercells of ABNNR for (a) Bare (b) One-edge PH_3 adsorption and (c) Both-edge PH_3 adsorption configurations. The Pink, blue, yellow and brown spheres correspond to B, N, P and H atoms respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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